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Magnetostructural Coupling in Oxides: Insights from First Principles

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Perovskite-structured transition metal oxides with ABO_3 stoichiometry display a myriad of useful phenomena, such as metal-insulator transitions, ferroelectricity, and superconductivity. These properties are due to their correlated electrons—the behavior of an electron depends explicitly on the location of all the others—and structural diversity. All oxides in this class, however, share a common flexible corner-connected oxygen octahedral network which makes their structural phase transitions dependent on temperature, pressure, and epitaxial strain. As a result of such structural changes, the allowed coupling between the magnetic and lattice degrees of freedom is determined from the modified crystal symmetry; the strength of the coupling is related to the angular modifications in the exchange pathways among the transitional metal oxygen bonds. In this talk, I illustrate how magnetostructural coupling in bulk perovskite oxides and heterostructures offers a new landscape for tailoring functionality. I describe how we combine first-principles (parameter-free) density functional theory (DFT) calculations with group theoretical tools and crystal chemistry to identify microscopic spin–lattice couplings by rational design. I conclude by outlining some open questions for engineering magnetostructural couplings and how high-resolution experimental probes could assist in identifying new control routes for these interactions.